



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:18 PM GMT

PDB ID : 1O9K  
Title : CRYSTAL STRUCTURE OF THE RETINOBLASTOMA TUMOUR SUPPRESSOR PROTEIN BOUND TO E2F PEPTIDE  
Authors : Xiao, B.; Spencer, J.; Clements, A.; Ali-Khan, N.; Mittnacht, S.; Broceno, C.; Burghammer, M.; Perrakis, A.; Marmorstein, R.; Gamblin, S.J.  
Deposited on : 2002-12-16  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

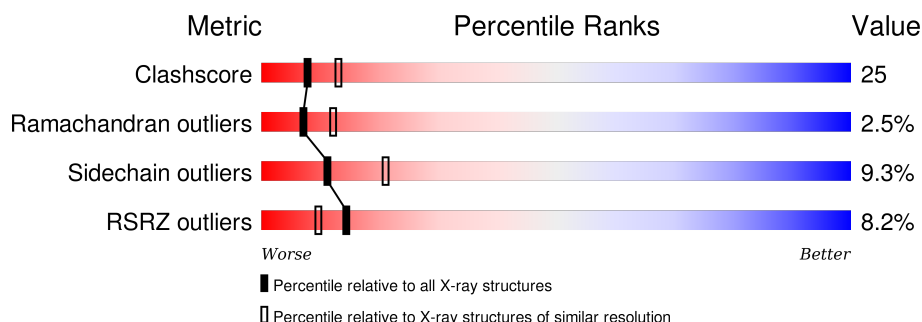
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	218	<div> <div>3%</div> <div>56% 27% 6% 11%</div> </div>
1	C	218	<div> <div>4%</div> <div>57% 25% 6% 11%</div> </div>
1	E	218	<div> <div>5%</div> <div>51% 31% 6% 11%</div> </div>
1	G	218	<div> <div>6%</div> <div>51% 32% 6% 11%</div> </div>
2	B	152	<div> <div>10%</div> <div>59% 31% 5% 5%</div> </div>
2	D	152	<div> <div>9%</div> <div>57% 34% 5%</div> </div>
2	F	152	<div> <div>11%</div> <div>56% 31% 7% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	152	<div><div></div><div>9%</div><div>48%</div><div>41%</div><div>6%</div><div>5%</div></div>
3	P	18	<div><div></div><div>22%</div><div>67%</div><div>22%</div><div>11%</div></div>
3	Q	18	<div><div></div><div>22%</div><div>50%</div><div>33%</div><div>11%</div><div>6%</div></div>
3	R	18	<div><div></div><div>33%</div><div>39%</div><div>33%</div><div>22%</div><div>6%</div></div>
3	S	18	<div><div></div><div>28%</div><div>39%</div><div>44%</div><div>17%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11974 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RETINOBLASTOMA-ASSOCIATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1569	1003	263	290	13			
1	C	194	Total	C	N	O	S	0	0	0
			1569	1003	263	290	13			
1	E	194	Total	C	N	O	S	0	0	0
			1569	1003	263	290	13			
1	G	194	Total	C	N	O	S	0	0	0
			1569	1003	263	290	13			

- Molecule 2 is a protein called RETINOBLASTOMA-ASSOCIATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	144	Total	C	N	O	S	0	0	0
			1213	789	205	211	8			
2	D	144	Total	C	N	O	S	0	0	0
			1213	789	205	211	8			
2	F	144	Total	C	N	O	S	0	0	0
			1213	789	205	211	8			
2	H	144	Total	C	N	O	S	0	0	0
			1213	789	205	211	8			

- Molecule 3 is a protein called TRANSCRIPTION FACTOR E2F1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	18	Total	C	N	O	0	0	0
			149	96	23	30			
3	Q	18	Total	C	N	O	0	0	0
			149	96	23	30			
3	R	18	Total	C	N	O	0	0	0
			149	96	23	30			
3	S	18	Total	C	N	O	0	0	0
			149	96	23	30			

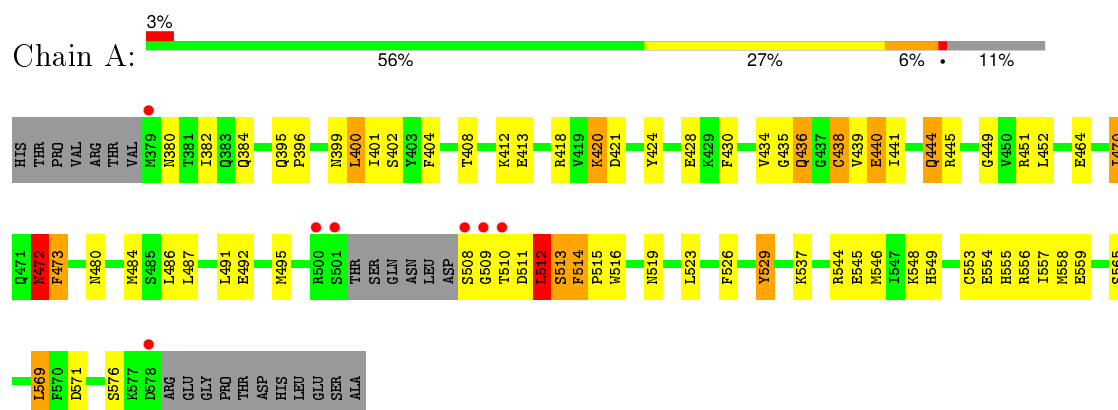
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	39	Total O 39 39	0	0
4	B	18	Total O 18 18	0	0
4	C	47	Total O 47 47	0	0
4	D	24	Total O 24 24	0	0
4	E	38	Total O 38 38	0	0
4	F	16	Total O 16 16	0	0
4	G	39	Total O 39 39	0	0
4	H	15	Total O 15 15	0	0
4	P	1	Total O 1 1	0	0
4	Q	4	Total O 4 4	0	0
4	R	4	Total O 4 4	0	0
4	S	5	Total O 5 5	0	0

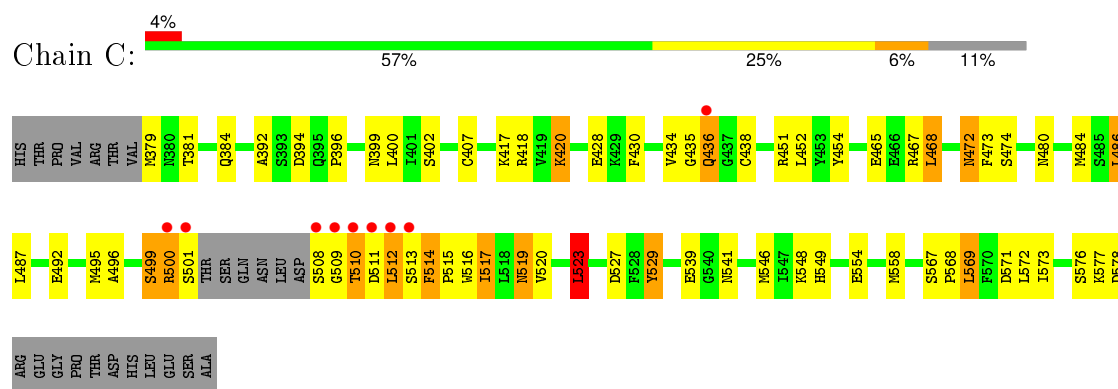
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

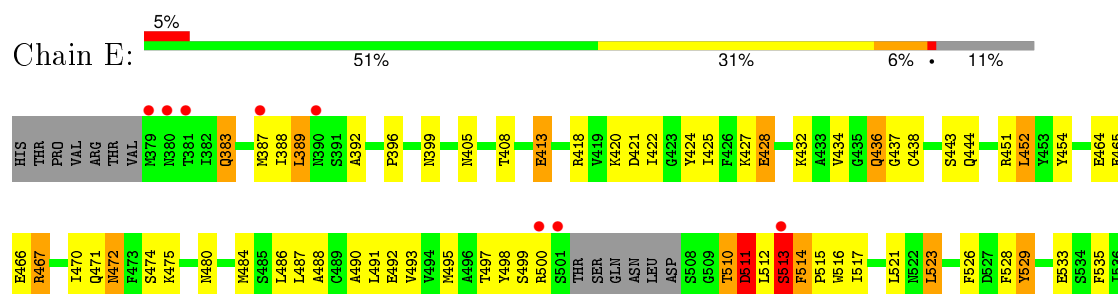
#### • Molecule 1: RETINOBLASTOMA-ASSOCIATED PROTEIN

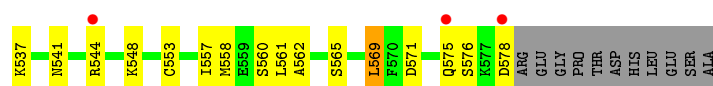


#### • Molecule 1: RETINOBLASTOMA-ASSOCIATED PROTEIN

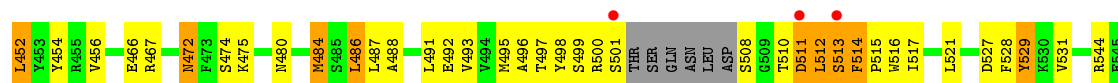


#### • Molecule 1: RETINOBLASTOMA-ASSOCIATED PROTEIN

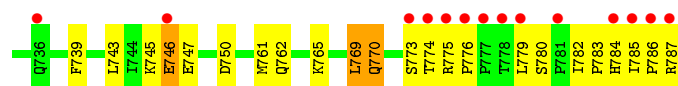




• Molecule 1: RETINOBLASTOMA-ASSOCIATED PROTEIN



• Molecule 2: RETINOBLASTOMA-ASSOCIATED PROTEIN



• Molecule 2: RETINOBLASTOMA-ASSOCIATED PROTEIN

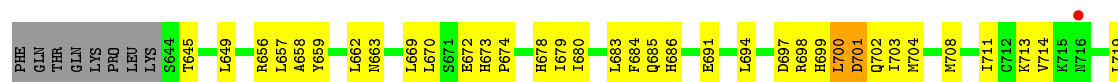


• Molecule 2: RETINOBLASTOMA-ASSOCIATED PROTEIN

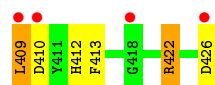


• Molecule 2: RETINOBLASTOMA-ASSOCIATED PROTEIN

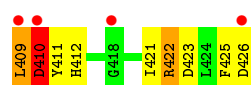




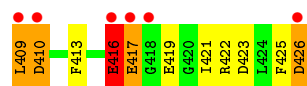
● Molecule 3: TRANSCRIPTION FACTOR E2F1



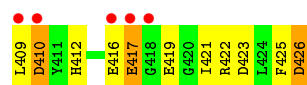
● Molecule 3: TRANSCRIPTION FACTOR E2F1



● Molecule 3: TRANSCRIPTION FACTOR E2F1



● Molecule 3: TRANSCRIPTION FACTOR E2F1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.00Å 158.55Å 110.62Å 90.00° 93.70° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.2 (20.00-2.60) 88.1 (19.82-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.80 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.229 , 0.285 0.228 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	18.3	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 47349 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	11974	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.55	0/1595	0.83	3/2141 (0.1%)
1	C	0.52	0/1595	0.81	5/2141 (0.2%)
1	E	0.52	0/1595	0.78	6/2141 (0.3%)
1	G	0.53	0/1595	0.77	5/2141 (0.2%)
2	B	0.46	0/1242	0.72	1/1680 (0.1%)
2	D	0.43	0/1242	0.72	2/1680 (0.1%)
2	F	0.39	0/1242	0.72	1/1680 (0.1%)
2	H	0.44	0/1242	0.73	3/1680 (0.2%)
3	P	0.47	0/152	0.91	1/203 (0.5%)
3	Q	0.40	0/152	0.83	1/203 (0.5%)
3	R	0.49	0/152	0.98	2/203 (1.0%)
3	S	0.42	0/152	0.87	1/203 (0.5%)
All	All	0.49	0/11956	0.77	31/16096 (0.2%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	GLY	N-CA-C	-9.23	90.02	113.10
1	A	571	ASP	CB-CG-OD2	6.71	124.34	118.30
1	C	468	LEU	N-CA-C	-6.58	93.24	111.00
2	H	730	ASP	CB-CG-OD2	6.32	123.99	118.30
2	H	701	ASP	CB-CG-OD2	6.17	123.85	118.30
1	C	527	ASP	CB-CG-OD2	6.15	123.84	118.30
1	E	523	LEU	CA-CB-CG	5.88	128.81	115.30
1	E	511	ASP	CB-CG-OD2	5.84	123.55	118.30
3	R	426	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	512	LEU	N-CA-C	5.71	126.41	111.00
1	E	513	SER	N-CA-C	-5.70	95.61	111.00
2	H	697	ASP	CB-CG-OD2	5.69	123.42	118.30
1	C	571	ASP	CB-CG-OD2	5.63	123.36	118.30
2	D	718	ASP	CB-CG-OD2	5.61	123.34	118.30
3	R	410	ASP	CB-CG-OD2	5.59	123.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	421	ASP	CB-CG-OD2	5.58	123.32	118.30
1	G	527	ASP	CB-CG-OD2	5.54	123.28	118.30
3	S	426	ASP	CB-CG-OD2	5.47	123.22	118.30
1	G	566	ASP	CB-CG-OD2	5.44	123.20	118.30
1	E	578	ASP	CB-CG-OD2	5.40	123.16	118.30
2	B	730	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	394	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	523	LEU	CB-CG-CD1	-5.22	102.12	111.00
1	G	513	SER	N-CA-C	-5.20	96.96	111.00
2	F	730	ASP	CB-CG-OD2	5.19	122.97	118.30
1	E	571	ASP	CB-CG-OD2	5.19	122.97	118.30
1	G	578	ASP	CB-CG-OD2	5.15	122.94	118.30
2	D	697	ASP	CB-CG-OD2	5.11	122.90	118.30
3	P	410	ASP	CB-CG-OD2	5.10	122.89	118.30
1	G	571	ASP	CB-CG-OD2	5.02	122.82	118.30
3	Q	410	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1569	0	1592	84	0
1	C	1569	0	1592	76	0
1	E	1569	0	1592	106	0
1	G	1569	0	1592	112	0
2	B	1213	0	1246	45	0
2	D	1213	0	1246	43	0
2	F	1213	0	1246	57	0
2	H	1213	0	1246	63	0
3	P	149	0	129	4	0
3	Q	149	0	129	11	0
3	R	149	0	129	17	0
3	S	149	0	129	10	0
4	A	39	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	18	0	0	3	0
4	C	47	0	0	14	0
4	D	24	0	0	1	0
4	E	38	0	0	8	0
4	F	16	0	0	3	0
4	G	39	0	0	9	0
4	H	15	0	0	8	0
4	P	1	0	0	0	0
4	Q	4	0	0	1	0
4	R	4	0	0	1	0
4	S	5	0	0	3	0
All	All	11974	0	11868	588	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (588) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LEU:HD22	1:A:512:LEU:O	1.28	1.27
1:C:513:SER:O	1:C:515:PRO:HD2	1.35	1.23
2:H:737:GLU:HB2	4:H:2008:HOH:O	1.36	1.21
1:C:509:GLY:HA2	4:C:2028:HOH:O	1.50	1.10
1:A:512:LEU:CD2	1:A:512:LEU:O	2.05	1.04
1:G:511:ASP:HB2	4:G:2025:HOH:O	1.55	1.04
1:G:514:PHE:HB2	1:G:553:CYS:SG	2.00	1.02
1:A:511:ASP:CG	1:A:512:LEU:H	1.61	0.96
1:G:428:GLU:HG3	1:G:432:LYS:NZ	1.81	0.96
1:G:495:MET:HG3	1:G:512:LEU:HG	1.50	0.94
1:E:493:VAL:O	1:E:497:THR:HG23	1.69	0.93
1:A:438:CYS:HG	1:G:438:CYS:HG	1.08	0.93
1:G:512:LEU:O	1:G:512:LEU:HD13	1.69	0.91
1:G:428:GLU:HG3	1:G:432:LYS:HZ2	1.35	0.91
1:G:493:VAL:O	1:G:497:THR:HG23	1.71	0.90
2:H:691:GLU:HB3	2:H:694:LEU:HD23	1.52	0.90
1:C:418:ARG:HH11	1:C:480:ASN:HD22	1.15	0.89
1:A:438:CYS:CB	1:G:438:CYS:HG	1.87	0.87
2:H:763:ARG:HD2	4:H:2013:HOH:O	1.74	0.87
2:F:761:MET:HG2	2:F:765:LYS:HE2	1.56	0.87
2:F:776:PRO:HB2	2:F:777:PRO:HD3	1.56	0.86
2:H:670:LEU:HD21	2:H:719:LEU:HD22	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:555:HIS:O	1:G:559:GLU:HG2	1.76	0.85
3:Q:410:ASP:HB3	4:Q:2001:HOH:O	1.76	0.84
1:C:509:GLY:CA	4:C:2028:HOH:O	2.17	0.83
2:F:741:ARG:NH2	4:F:2013:HOH:O	2.10	0.83
1:E:514:PHE:N	1:E:515:PRO:CD	2.41	0.83
1:E:513:SER:HB2	1:E:515:PRO:HD2	1.58	0.82
1:C:492:GLU:OE1	1:C:512:LEU:HD11	1.80	0.82
1:E:512:LEU:C	1:E:512:LEU:HD13	2.00	0.82
2:F:714:VAL:HG21	2:F:768:ILE:CG2	2.09	0.82
1:A:513:SER:O	1:A:515:PRO:HD2	1.81	0.81
2:H:679:ILE:HG22	2:H:711:ILE:HD13	1.61	0.81
2:F:680:ILE:HA	2:F:711:ILE:HD12	1.61	0.80
1:A:512:LEU:O	1:A:513:SER:C	2.19	0.80
2:H:680:ILE:HA	2:H:711:ILE:HD12	1.62	0.80
1:C:519:ASN:HB3	4:C:2031:HOH:O	1.80	0.79
2:H:764:LEU:O	2:H:768:ILE:HG13	1.82	0.79
1:E:418:ARG:HH11	1:E:480:ASN:HD22	1.30	0.78
1:E:537:LYS:HG2	3:R:413:PHE:HE2	1.46	0.78
2:B:776:PRO:HG2	4:B:2018:HOH:O	1.84	0.78
1:E:512:LEU:O	1:E:512:LEU:HD13	1.84	0.78
1:A:554:GLU:HG2	1:A:558:MET:HE2	1.66	0.78
1:E:428:GLU:HB3	1:E:432:LYS:NZ	1.99	0.78
1:A:512:LEU:C	1:A:512:LEU:HD13	2.04	0.77
1:A:472:ASN:O	1:A:473:PHE:HB2	1.84	0.77
2:D:765:LYS:O	2:D:769:LEU:HD23	1.83	0.76
1:A:519:ASN:HB3	4:A:2023:HOH:O	1.86	0.76
2:F:785:ILE:HG22	2:F:787:ARG:HH11	1.50	0.76
2:H:765:LYS:O	2:H:769:LEU:HD23	1.85	0.76
1:E:513:SER:CB	1:E:515:PRO:HD2	2.16	0.76
1:A:451:ARG:HH22	1:G:508:SER:HB2	1.50	0.75
1:E:470:ILE:HG22	1:E:472:ASN:H	1.50	0.75
2:H:714:VAL:HG11	2:H:768:ILE:HG22	1.68	0.75
1:C:512:LEU:HA	1:C:516:TRP:HB3	1.68	0.75
1:E:436:GLN:HG3	4:E:2019:HOH:O	1.86	0.75
1:C:492:GLU:CD	1:C:512:LEU:HD11	2.08	0.74
1:G:513:SER:C	1:G:515:PRO:HD2	2.08	0.74
2:F:771:TYR:HA	2:F:776:PRO:HB3	1.70	0.73
2:F:714:VAL:HG21	2:F:768:ILE:HG22	1.69	0.73
2:H:787:ARG:HG3	2:H:787:ARG:HH11	1.54	0.73
3:Q:422:ARG:O	3:Q:426:ASP:HB2	1.87	0.72
1:C:501:SER:HA	4:C:2027:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:GLU:HG3	1:E:424:TYR:HE2	1.54	0.71
2:H:784:HIS:O	2:H:786:PRO:HD3	1.90	0.71
1:A:511:ASP:CG	1:A:512:LEU:N	2.37	0.71
1:G:512:LEU:HD22	1:G:513:SER:O	1.91	0.71
2:F:776:PRO:HD2	2:F:777:PRO:HD2	1.73	0.71
1:A:546:MET:HE3	1:A:549:HIS:HB3	1.73	0.70
3:S:416:GLU:HB2	3:S:419:GLU:HG3	1.72	0.70
2:F:737:GLU:HB2	4:F:2011:HOH:O	1.91	0.70
1:A:382:ILE:HD12	4:A:2037:HOH:O	1.91	0.70
2:H:746:GLU:HG2	2:H:747:GLU:H	1.56	0.70
1:E:514:PHE:N	1:E:515:PRO:HD2	2.06	0.70
2:B:660:LEU:HD11	2:B:785:ILE:HD11	1.72	0.70
1:A:556:ARG:HA	1:A:559:GLU:HG2	1.74	0.70
2:H:703:ILE:N	2:H:703:ILE:HD12	2.07	0.70
1:G:512:LEU:C	1:G:512:LEU:HD13	2.12	0.69
1:A:445:ARG:NE	4:A:2010:HOH:O	2.18	0.69
1:G:512:LEU:CD1	1:G:512:LEU:O	2.39	0.69
2:D:678:HIS:ND1	2:D:779:LEU:HD13	2.08	0.69
1:E:436:GLN:NE2	4:E:2018:HOH:O	2.25	0.69
1:A:556:ARG:CZ	4:A:2032:HOH:O	2.39	0.69
1:G:512:LEU:HD22	1:G:516:TRP:HB3	1.75	0.69
3:Q:409:LEU:C	3:Q:411:TYR:H	1.95	0.69
1:E:514:PHE:C	1:E:514:PHE:CD2	2.66	0.69
1:G:514:PHE:N	1:G:515:PRO:CD	2.56	0.69
2:F:680:ILE:HA	2:F:711:ILE:CD1	2.23	0.69
1:G:512:LEU:CD2	1:G:516:TRP:HB3	2.23	0.68
1:G:428:GLU:CG	1:G:432:LYS:NZ	2.55	0.68
2:H:678:HIS:HE1	2:H:780:SER:O	1.76	0.68
2:F:735:VAL:HG12	2:F:737:GLU:H	1.58	0.68
2:B:668:ARG:HB3	1:C:500:ARG:HG3	1.74	0.68
1:G:495:MET:HB2	1:G:512:LEU:HD12	1.76	0.68
1:E:514:PHE:HB2	1:E:553:CYS:SG	2.34	0.67
1:E:511:ASP:OD1	1:E:512:LEU:N	2.26	0.67
2:B:668:ARG:HD3	1:C:500:ARG:NH1	2.09	0.67
1:C:435:GLY:H	1:C:508:SER:HA	1.58	0.67
1:C:436:GLN:N	1:C:436:GLN:HE21	1.92	0.67
1:C:407:CYS:HA	1:C:472:ASN:ND2	2.10	0.67
1:C:492:GLU:OE2	1:C:512:LEU:HD11	1.95	0.67
1:E:492:GLU:OE2	1:E:512:LEU:HD11	1.94	0.67
1:C:548:LYS:HD2	4:C:2040:HOH:O	1.94	0.67
1:E:513:SER:C	1:E:515:PRO:HD2	2.15	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:508:SER:N	1:G:513:SER:HG	1.93	0.67
1:A:495:MET:CE	1:A:512:LEU:HB2	2.26	0.66
1:G:546:MET:HE3	1:G:549:HIS:HB3	1.77	0.66
1:E:565:SER:OG	2:F:697:ASP:OD2	2.13	0.66
2:H:763:ARG:CD	4:H:2013:HOH:O	2.38	0.66
3:Q:409:LEU:O	3:Q:411:TYR:N	2.28	0.66
2:B:668:ARG:O	1:C:500:ARG:HB2	1.95	0.66
1:E:514:PHE:O	1:E:514:PHE:CD2	2.48	0.66
2:B:656:ARG:NH1	3:P:412:HIS:HB2	2.09	0.66
2:H:698:ARG:HG2	4:H:2010:HOH:O	1.94	0.66
1:E:472:ASN:HD22	1:E:472:ASN:C	1.99	0.65
2:D:746:GLU:H	2:D:746:GLU:CD	1.99	0.65
1:C:418:ARG:HH11	1:C:480:ASN:ND2	1.91	0.65
2:F:656:ARG:NH2	4:F:2001:HOH:O	2.29	0.65
2:B:676:LEU:HD11	2:B:717:ILE:HG13	1.77	0.65
1:G:510:THR:O	1:G:512:LEU:N	2.30	0.65
1:G:577:LYS:O	4:G:2039:HOH:O	2.14	0.65
2:D:745:LYS:HB2	2:D:746:GLU:OE2	1.97	0.65
1:E:418:ARG:NH1	1:E:480:ASN:HD22	1.93	0.64
2:D:775:ARG:HB2	2:D:776:PRO:HD2	1.79	0.64
2:F:710:GLY:O	2:F:714:VAL:HG23	1.96	0.64
1:C:418:ARG:NH1	1:C:480:ASN:HD22	1.93	0.64
2:F:784:HIS:CD2	2:F:786:PRO:HG2	2.31	0.64
2:F:776:PRO:CB	2:F:777:PRO:HD3	2.27	0.64
1:G:513:SER:CB	1:G:515:PRO:HD2	2.26	0.64
2:D:785:ILE:HG22	2:D:785:ILE:O	1.98	0.64
1:A:492:GLU:OE1	1:A:512:LEU:HD21	1.98	0.64
1:A:440:GLU:HG2	1:G:434:VAL:HG11	1.78	0.64
1:G:418:ARG:HH11	1:G:480:ASN:HD22	1.45	0.63
1:C:465:GLU:O	1:C:468:LEU:O	2.16	0.63
1:G:510:THR:C	1:G:512:LEU:H	2.02	0.63
1:E:495:MET:HB3	1:E:512:LEU:CB	2.28	0.63
2:B:785:ILE:O	2:B:785:ILE:HG23	1.99	0.63
1:A:472:ASN:O	1:A:473:PHE:CB	2.47	0.62
2:F:659:TYR:HB2	2:F:783:PRO:HG2	1.81	0.62
1:A:438:CYS:HB2	1:G:438:CYS:HG	1.64	0.62
1:C:428:GLU:CD	4:C:2018:HOH:O	2.38	0.62
2:B:775:ARG:NH1	4:B:2017:HOH:O	2.31	0.62
1:G:512:LEU:HD23	1:G:516:TRP:HE3	1.63	0.62
1:A:438:CYS:HB2	1:G:438:CYS:SG	2.40	0.62
1:A:556:ARG:NE	4:A:2032:HOH:O	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:761:MET:HG2	2:B:762:GLN:NE2	2.14	0.61
1:G:495:MET:HB3	1:G:512:LEU:HB3	1.82	0.61
2:F:725:VAL:O	2:F:729:LYS:HG3	1.99	0.61
1:E:383:GLN:O	1:E:387:MET:HG2	2.00	0.61
1:A:408:THR:H	1:A:472:ASN:HD21	1.49	0.61
2:D:746:GLU:CD	2:D:746:GLU:N	2.54	0.61
3:S:409:LEU:O	3:S:410:ASP:HB3	2.00	0.61
1:G:472:ASN:HD21	1:G:474:SER:HB2	1.66	0.61
2:D:662:LEU:HD22	2:D:666:CYS:SG	2.40	0.61
2:F:776:PRO:HB2	2:F:777:PRO:CD	2.28	0.61
1:A:512:LEU:O	1:A:512:LEU:CG	2.48	0.60
1:G:420:LYS:HD3	4:G:2014:HOH:O	2.01	0.60
2:D:773:SER:OG	2:D:775:ARG:HG2	2.01	0.60
1:G:500:ARG:NE	1:G:500:ARG:HA	2.15	0.60
1:G:500:ARG:HE	1:G:500:ARG:N	1.98	0.60
1:A:399:ASN:O	1:A:402:SER:HB3	2.01	0.60
2:D:672:GLU:C	2:D:674:PRO:HD3	2.22	0.60
2:H:691:GLU:HB3	2:H:694:LEU:CD2	2.30	0.60
3:Q:421:ILE:HD11	3:Q:425:PHE:HE1	1.67	0.60
1:G:383:GLN:O	1:G:387:MET:HG3	2.02	0.60
1:A:418:ARG:HH11	1:A:480:ASN:HD22	1.50	0.60
3:R:409:LEU:HD12	3:R:410:ASP:CB	2.31	0.60
1:E:512:LEU:CD1	1:E:512:LEU:O	2.49	0.60
1:G:472:ASN:HD22	1:G:472:ASN:C	2.05	0.60
1:C:472:ASN:C	1:C:472:ASN:ND2	2.54	0.59
1:G:396:PRO:HD3	1:G:454:TYR:CZ	2.37	0.59
1:E:475:LYS:NZ	3:R:426:ASP:HA	2.17	0.59
1:E:427:LYS:HE2	1:E:443:SER:HA	1.83	0.59
2:F:673:HIS:N	2:F:674:PRO:HD3	2.18	0.59
2:B:773:SER:OG	2:B:775:ARG:HG2	2.02	0.59
1:G:499:SER:HB3	4:G:2025:HOH:O	2.03	0.59
1:A:424:TYR:OH	1:E:428:GLU:HG2	2.01	0.59
1:G:432:LYS:CG	4:G:2015:HOH:O	2.51	0.59
2:D:656:ARG:HD2	3:Q:412:HIS:CD2	2.37	0.59
1:G:500:ARG:H	1:G:500:ARG:HE	1.49	0.59
2:F:746:GLU:HG2	2:F:747:GLU:N	2.17	0.59
1:C:472:ASN:HD21	1:C:474:SER:HB2	1.68	0.59
1:E:569:LEU:O	1:E:569:LEU:HD22	2.03	0.59
1:A:413:GLU:HA	1:A:413:GLU:OE1	2.02	0.59
2:F:676:LEU:O	2:F:680:ILE:HG13	2.03	0.58
2:H:745:LYS:NZ	2:H:746:GLU:OE2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:746:GLU:HG2	2:D:747:GLU:H	1.68	0.58
2:D:691:GLU:HG3	2:D:764:LEU:HD21	1.85	0.58
2:H:770:GLN:HB3	2:H:777:PRO:HD3	1.85	0.58
2:B:678:HIS:HD2	2:B:779:LEU:HD13	1.68	0.58
2:F:678:HIS:CE1	2:F:779:LEU:HB3	2.38	0.58
1:E:413:GLU:CG	4:E:2010:HOH:O	2.50	0.58
2:D:769:LEU:O	2:D:772:ALA:HB3	2.04	0.58
2:D:676:LEU:HD11	2:D:717:ILE:HG13	1.85	0.58
1:A:512:LEU:O	1:A:512:LEU:HD13	2.03	0.58
2:D:691:GLU:O	2:D:694:LEU:HD23	2.04	0.58
3:S:421:ILE:HD11	3:S:425:PHE:HE1	1.69	0.58
1:E:512:LEU:CD1	1:E:512:LEU:C	2.70	0.57
1:C:467:ARG:CZ	1:C:468:LEU:HD21	2.34	0.57
2:D:770:GLN:HG3	4:D:2023:HOH:O	2.03	0.57
1:G:510:THR:C	1:G:512:LEU:N	2.56	0.57
2:F:746:GLU:HG2	2:F:747:GLU:H	1.69	0.57
1:E:510:THR:O	1:E:511:ASP:C	2.41	0.57
3:R:410:ASP:O	3:R:410:ASP:CG	2.41	0.57
2:B:746:GLU:N	2:B:746:GLU:CD	2.57	0.57
1:A:440:GLU:HA	1:G:434:VAL:CG1	2.34	0.57
2:H:763:ARG:NH2	4:H:2011:HOH:O	2.36	0.57
1:E:512:LEU:HD22	1:E:516:TRP:HB3	1.85	0.57
1:E:498:TYR:C	1:E:500:ARG:H	2.06	0.57
1:E:420:LYS:C	1:E:420:LYS:HD3	2.25	0.57
1:E:388:ILE:HG23	1:E:541:ASN:HD22	1.70	0.57
1:C:512:LEU:C	1:C:512:LEU:HD13	2.25	0.57
1:E:495:MET:HB3	1:E:512:LEU:HB3	1.87	0.57
2:D:699:HIS:HB3	2:D:702:GLN:HG3	1.85	0.57
3:Q:409:LEU:HD23	3:Q:409:LEU:N	2.20	0.57
1:G:388:ILE:HG22	1:G:388:ILE:O	2.02	0.57
1:E:418:ARG:HH11	1:E:480:ASN:ND2	1.99	0.56
1:G:500:ARG:NE	1:G:500:ARG:CA	2.68	0.56
3:R:409:LEU:HD12	3:R:410:ASP:N	2.20	0.56
1:G:528:PHE:O	1:G:531:VAL:HG12	2.05	0.56
1:G:514:PHE:N	1:G:515:PRO:HD2	2.20	0.56
1:E:512:LEU:HD22	1:E:513:SER:O	2.05	0.56
1:E:495:MET:HB2	1:E:512:LEU:HG	1.87	0.56
1:A:464:GLU:HA	1:A:464:GLU:OE1	2.05	0.56
2:H:645:THR:HG23	3:S:419:GLU:OE1	2.03	0.56
2:H:703:ILE:N	2:H:703:ILE:CD1	2.68	0.56
2:H:656:ARG:HH21	2:H:785:ILE:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:GLU:HA	1:G:434:VAL:HG13	1.86	0.56
1:A:513:SER:O	1:A:515:PRO:CD	2.54	0.56
1:C:514:PHE:O	1:C:515:PRO:C	2.43	0.56
1:E:464:GLU:HA	1:E:464:GLU:OE1	2.06	0.56
1:G:492:GLU:OE1	1:G:512:LEU:HD11	2.05	0.56
2:H:694:LEU:HD21	2:H:763:ARG:HG2	1.87	0.56
1:A:428:GLU:HG3	1:E:424:TYR:CE2	2.38	0.56
1:C:516:TRP:O	1:C:520:VAL:HG23	2.06	0.55
1:E:392:ALA:O	1:E:451:ARG:HD2	2.06	0.55
2:H:783:PRO:O	2:H:785:ILE:HG13	2.06	0.55
2:D:701:ASP:OD2	2:D:733:HIS:HE1	1.88	0.55
2:D:673:HIS:N	2:D:674:PRO:HD3	2.21	0.55
2:H:699:HIS:HB3	2:H:702:GLN:HG3	1.88	0.55
3:R:416:GLU:HB2	3:R:419:GLU:OE2	2.06	0.55
1:E:510:THR:O	1:E:511:ASP:O	2.24	0.55
1:E:389:LEU:O	1:E:451:ARG:NH1	2.39	0.55
2:F:662:LEU:HD22	2:F:666:CYS:SG	2.46	0.55
1:A:435:GLY:HA2	1:A:508:SER:N	2.21	0.55
1:A:438:CYS:CB	1:G:438:CYS:SG	2.92	0.55
1:A:430:PHE:CE1	1:A:434:VAL:HG21	2.41	0.55
1:G:514:PHE:O	1:G:514:PHE:CD2	2.59	0.55
1:A:401:ILE:HD12	1:A:412:LYS:HD2	1.88	0.55
2:H:787:ARG:HG3	2:H:787:ARG:NH1	2.22	0.55
1:A:508:SER:HA	4:A:2020:HOH:O	2.06	0.54
1:G:428:GLU:CG	1:G:432:LYS:HZ1	2.19	0.54
1:E:472:ASN:ND2	1:E:474:SER:H	2.04	0.54
1:A:382:ILE:CD1	4:A:2037:HOH:O	2.51	0.54
3:S:409:LEU:O	3:S:410:ASP:CB	2.55	0.54
2:H:673:HIS:N	2:H:674:PRO:HD3	2.22	0.54
1:G:495:MET:CG	1:G:512:LEU:HG	2.32	0.54
1:G:514:PHE:CB	1:G:553:CYS:SG	2.86	0.54
3:Q:423:ASP:HA	3:Q:426:ASP:CB	2.37	0.54
2:B:678:HIS:HE1	2:B:780:SER:O	1.90	0.54
2:B:765:LYS:HB2	2:B:765:LYS:NZ	2.21	0.54
2:B:678:HIS:CD2	2:B:779:LEU:HD13	2.41	0.54
2:B:725:VAL:HG13	2:B:739:PHE:CZ	2.42	0.54
1:G:387:MET:O	1:G:389:LEU:N	2.40	0.54
1:C:558:MET:HB3	2:D:654:VAL:HG22	1.88	0.54
1:C:569:LEU:HD22	1:C:573:ILE:HG13	1.88	0.54
2:F:663:ASN:O	2:F:667:GLU:HG3	2.08	0.54
1:C:379:MET:N	4:C:2001:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:ASN:C	1:C:472:ASN:HD22	2.11	0.54
1:C:529:TYR:OH	2:D:649:LEU:HD12	2.08	0.54
1:A:435:GLY:O	1:A:436:GLN:HG3	2.08	0.54
2:B:745:LYS:HB3	2:B:746:GLU:OE1	2.09	0.53
1:G:449:GLY:HA3	1:G:491:LEU:HD23	1.90	0.53
2:H:725:VAL:O	2:H:729:LYS:HG3	2.09	0.53
1:A:512:LEU:CD1	1:A:512:LEU:O	2.57	0.53
2:B:678:HIS:CE1	2:B:780:SER:O	2.61	0.53
1:C:430:PHE:O	1:C:434:VAL:HG23	2.09	0.53
1:E:388:ILE:HD12	1:E:541:ASN:HB3	1.90	0.53
1:G:475:LYS:HD3	4:S:2005:HOH:O	2.09	0.53
2:F:785:ILE:N	2:F:786:PRO:HD2	2.24	0.53
3:S:422:ARG:O	3:S:426:ASP:HB2	2.09	0.53
1:G:514:PHE:HB2	1:G:553:CYS:HG	1.68	0.53
2:B:783:PRO:O	2:B:785:ILE:HG22	2.09	0.53
3:Q:423:ASP:HA	3:Q:426:ASP:HB3	1.90	0.52
1:C:420:LYS:HE2	4:C:2015:HOH:O	2.08	0.52
1:C:546:MET:HE3	1:C:549:HIS:HB3	1.90	0.52
1:E:488:ALA:HB2	1:E:521:LEU:HD12	1.90	0.52
2:B:773:SER:C	2:B:775:ARG:H	2.13	0.52
2:B:691:GLU:O	2:B:694:LEU:HB2	2.09	0.52
1:E:413:GLU:HG2	4:E:2010:HOH:O	2.10	0.52
1:G:452:LEU:O	1:G:456:VAL:HG23	2.10	0.52
1:A:434:VAL:O	1:A:435:GLY:C	2.47	0.52
1:G:418:ARG:NH1	1:G:480:ASN:HD22	2.08	0.52
1:G:407:CYS:HA	1:G:472:ASN:ND2	2.25	0.52
3:R:409:LEU:HD12	3:R:409:LEU:C	2.30	0.52
1:A:435:GLY:HA2	4:A:2019:HOH:O	2.09	0.52
1:A:512:LEU:CD1	1:A:512:LEU:C	2.69	0.52
1:G:432:LYS:HG2	4:G:2015:HOH:O	2.10	0.52
1:E:472:ASN:ND2	1:E:472:ASN:C	2.62	0.52
2:D:660:LEU:HD21	2:D:785:ILE:HD13	1.93	0.52
1:A:444:GLN:HE22	1:G:510:THR:HG22	1.75	0.51
2:B:680:ILE:HD13	2:B:708:MET:HA	1.92	0.51
1:A:544:ARG:CZ	1:A:545:GLU:OE2	2.59	0.51
3:P:422:ARG:O	3:P:426:ASP:HB2	2.09	0.51
2:F:784:HIS:NE2	2:F:786:PRO:HG2	2.25	0.51
1:E:383:GLN:HE21	1:E:383:GLN:HA	1.76	0.51
1:C:554:GLU:O	1:C:558:MET:HE2	2.10	0.51
1:E:557:ILE:HA	1:E:561:LEU:HB2	1.91	0.51
2:H:686:HIS:NE2	2:H:767:ASN:ND2	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:511:ASP:HB3	4:G:2024:HOH:O	2.11	0.51
1:G:436:GLN:N	1:G:436:GLN:HE21	2.09	0.51
2:H:704:MET:O	2:H:708:MET:HG3	2.11	0.51
2:B:761:MET:HG2	2:B:762:GLN:HE21	1.74	0.51
1:E:405:ASN:ND2	4:E:2009:HOH:O	2.39	0.51
1:E:472:ASN:HD21	1:E:474:SER:HB2	1.74	0.50
2:D:691:GLU:HB3	2:D:694:LEU:CD2	2.41	0.50
1:A:545:GLU:N	1:A:545:GLU:CD	2.65	0.50
2:F:672:GLU:C	2:F:674:PRO:HD3	2.31	0.50
2:D:676:LEU:O	2:D:680:ILE:HG13	2.11	0.50
1:E:498:TYR:C	1:E:500:ARG:N	2.64	0.50
1:A:400:LEU:HD22	1:A:404:PHE:CE1	2.46	0.50
1:C:436:GLN:N	1:C:436:GLN:NE2	2.57	0.50
1:E:428:GLU:CB	1:E:432:LYS:NZ	2.73	0.50
2:H:745:LYS:HB3	2:H:745:LYS:NZ	2.26	0.50
2:B:725:VAL:HG12	2:B:726:THR:N	2.26	0.50
2:H:669:LEU:HD11	2:H:727:ALA:CB	2.42	0.50
1:G:514:PHE:C	1:G:514:PHE:CD2	2.85	0.50
1:G:475:LYS:HE3	4:S:2005:HOH:O	2.12	0.50
1:G:544:ARG:HH11	1:G:544:ARG:HG2	1.76	0.50
1:A:421:ASP:HB3	1:E:425:ILE:CD1	2.42	0.50
1:A:495:MET:HE1	1:A:512:LEU:HB2	1.94	0.49
1:C:399:ASN:O	1:C:402:SER:HB3	2.12	0.49
1:G:491:LEU:O	1:G:495:MET:HG2	2.12	0.49
2:D:704:MET:O	2:D:708:MET:HG3	2.13	0.49
3:Q:409:LEU:C	3:Q:411:TYR:N	2.64	0.49
1:E:523:LEU:CD1	1:E:528:PHE:HB2	2.42	0.49
1:E:396:PRO:HD3	1:E:454:TYR:CZ	2.47	0.49
1:A:495:MET:HE2	1:A:512:LEU:HB2	1.93	0.49
1:E:558:MET:SD	2:F:653:LYS:HB3	2.52	0.49
1:E:452:LEU:HD11	1:E:535:PHE:HZ	1.75	0.49
1:E:452:LEU:HD12	1:E:490:ALA:HA	1.95	0.49
2:B:698:ARG:HG2	4:B:2010:HOH:O	2.12	0.49
1:E:544:ARG:HG2	1:E:544:ARG:HH11	1.78	0.49
1:E:465:GLU:OE1	1:E:471:GLN:HG3	2.11	0.49
1:C:509:GLY:C	4:C:2029:HOH:O	2.51	0.49
2:F:774:THR:O	2:F:775:ARG:HB2	2.12	0.49
2:D:691:GLU:O	2:D:694:LEU:CD2	2.61	0.49
2:H:787:ARG:HD2	2:H:787:ARG:N	2.27	0.49
2:F:776:PRO:CB	2:F:777:PRO:CD	2.87	0.49
2:F:679:ILE:HG22	2:F:711:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:736:GLN:HA	2:H:739:PHE:CE2	2.48	0.49
2:H:748:GLU:HA	2:H:748:GLU:OE1	2.13	0.49
1:G:512:LEU:HD23	1:G:516:TRP:HB3	1.94	0.49
1:C:548:LYS:CD	4:C:2040:HOH:O	2.59	0.49
2:H:686:HIS:HE2	2:H:767:ASN:ND2	2.11	0.49
2:B:679:ILE:HG22	2:B:711:ILE:HG12	1.95	0.49
2:H:746:GLU:HG2	2:H:747:GLU:N	2.27	0.49
1:A:553:CYS:O	1:A:557:ILE:HG13	2.13	0.49
1:A:408:THR:O	2:F:696:ARG:NH2	2.44	0.48
1:G:557:ILE:HA	1:G:561:LEU:HB2	1.95	0.48
1:A:513:SER:C	1:A:515:PRO:HD2	2.34	0.48
2:H:703:ILE:H	2:H:703:ILE:CD1	2.26	0.48
2:B:676:LEU:O	2:B:680:ILE:HG13	2.13	0.48
1:A:565:SER:OG	2:B:697:ASP:OD2	2.31	0.48
1:A:439:VAL:O	1:A:441:ILE:N	2.46	0.48
1:C:509:GLY:N	4:C:2029:HOH:O	2.47	0.48
1:G:434:VAL:HG12	1:G:434:VAL:O	2.12	0.48
2:H:745:LYS:O	2:H:746:GLU:C	2.51	0.48
2:H:656:ARG:HE	2:H:785:ILE:HG12	1.78	0.48
1:G:513:SER:C	1:G:515:PRO:CD	2.80	0.48
1:A:555:HIS:HD2	1:A:558:MET:HE1	1.79	0.48
2:H:656:ARG:HD2	3:S:412:HIS:CD2	2.48	0.48
1:A:435:GLY:N	1:A:508:SER:O	2.47	0.48
1:E:491:LEU:O	1:E:495:MET:HG2	2.13	0.48
1:C:513:SER:O	1:C:514:PHE:HB3	2.12	0.48
2:H:745:LYS:HB3	2:H:745:LYS:HZ3	1.79	0.48
1:E:388:ILE:HD12	1:E:541:ASN:CB	2.43	0.48
1:G:393:SER:O	1:G:451:ARG:HG2	2.13	0.48
2:F:785:ILE:N	2:F:786:PRO:CD	2.77	0.48
1:G:472:ASN:ND2	1:G:474:SER:H	2.11	0.47
1:C:539:GLU:OE2	1:C:541:ASN:HB2	2.14	0.47
1:C:514:PHE:CD2	1:C:514:PHE:C	2.85	0.47
1:G:467:ARG:NH2	3:S:423:ASP:OD2	2.47	0.47
2:F:743:LEU:HD23	2:F:749:TYR:CZ	2.49	0.47
2:H:701:ASP:OD2	2:H:733:HIS:HE1	1.97	0.47
1:G:428:GLU:CG	1:G:432:LYS:HZ2	2.15	0.47
1:E:512:LEU:HD13	1:E:513:SER:O	2.14	0.47
2:B:784:HIS:O	2:B:785:ILE:HG22	2.13	0.47
1:G:480:ASN:HD21	1:G:484:MET:CE	2.27	0.47
1:A:449:GLY:HA3	1:A:491:LEU:HD23	1.96	0.47
2:F:776:PRO:HD2	2:F:777:PRO:CD	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:495:MET:CB	1:E:512:LEU:HG	2.44	0.47
1:E:513:SER:C	1:E:515:PRO:CD	2.81	0.47
1:E:444:GLN:HG3	4:E:2025:HOH:O	2.14	0.47
1:E:513:SER:O	1:E:514:PHE:C	2.52	0.47
1:C:472:ASN:HD22	1:C:473:PHE:N	2.13	0.47
1:G:500:ARG:HB2	4:G:2021:HOH:O	2.15	0.47
2:D:693:GLU:OE2	2:D:696:ARG:NH1	2.48	0.47
1:A:514:PHE:C	1:A:514:PHE:CD2	2.84	0.47
1:E:514:PHE:HB2	1:E:553:CYS:HG	1.78	0.47
1:G:500:ARG:CA	1:G:500:ARG:HE	2.28	0.47
1:E:475:LYS:HZ1	3:R:426:ASP:C	2.17	0.47
2:H:684:PHE:HZ	2:H:700:LEU:HD22	1.80	0.47
2:B:769:LEU:O	2:B:770:GLN:C	2.54	0.47
1:A:512:LEU:HD13	1:A:513:SER:N	2.30	0.47
1:E:557:ILE:HG22	1:E:562:ALA:HB2	1.97	0.47
1:C:511:ASP:O	1:C:512:LEU:C	2.53	0.46
1:G:488:ALA:HB2	1:G:521:LEU:HD12	1.96	0.46
2:B:678:HIS:CD2	2:B:779:LEU:HB3	2.50	0.46
1:E:464:GLU:OE1	1:E:467:ARG:NH1	2.48	0.46
1:A:420:LYS:O	1:A:420:LYS:HE2	2.14	0.46
1:E:408:THR:H	1:E:474:SER:HB2	1.80	0.46
2:H:669:LEU:HD11	2:H:727:ALA:HB2	1.97	0.46
1:G:492:GLU:CD	1:G:512:LEU:HD11	2.36	0.46
2:F:773:SER:O	2:F:776:PRO:HG3	2.15	0.46
1:C:495:MET:HE2	1:C:512:LEU:CB	2.45	0.46
1:G:511:ASP:O	1:G:512:LEU:HB2	2.16	0.46
2:B:660:LEU:HD11	2:B:785:ILE:CD1	2.42	0.46
1:E:452:LEU:CD1	1:E:535:PHE:HZ	2.27	0.46
2:B:699:HIS:HB3	2:B:702:GLN:HG3	1.98	0.46
1:C:514:PHE:HB3	1:C:515:PRO:CD	2.45	0.46
2:D:675:GLU:N	2:D:675:GLU:OE1	2.35	0.46
1:C:495:MET:HE2	1:C:512:LEU:HB2	1.98	0.46
3:R:419:GLU:HA	3:R:423:ASP:OD2	2.16	0.46
1:C:554:GLU:HG2	1:C:558:MET:CE	2.46	0.46
1:E:432:LYS:HE2	1:G:432:LYS:HD3	1.97	0.46
3:R:421:ILE:HD11	3:R:425:PHE:HE1	1.81	0.46
2:B:656:ARG:HG2	2:B:785:ILE:HD12	1.98	0.45
1:C:435:GLY:O	1:C:436:GLN:HG3	2.16	0.45
1:G:472:ASN:HD22	1:G:474:SER:H	1.63	0.45
2:B:710:GLY:O	2:B:713:LYS:HB2	2.16	0.45
1:C:381:THR:O	1:C:384:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:714:VAL:HG13	4:H:2005:HOH:O	2.15	0.45
2:D:653:LYS:HD3	3:Q:412:HIS:CD2	2.52	0.45
2:H:658:ALA:HB1	2:H:684:PHE:CE2	2.51	0.45
1:C:392:ALA:O	1:C:451:ARG:HD3	2.16	0.45
1:G:418:ARG:O	1:G:422:ILE:HG12	2.16	0.45
1:G:452:LEU:HD22	1:G:456:VAL:HG23	1.97	0.45
1:E:533:GLU:O	1:E:537:LYS:HG3	2.17	0.45
2:D:678:HIS:CE1	2:D:779:LEU:HB3	2.52	0.45
2:B:746:GLU:H	2:B:746:GLU:CD	2.20	0.45
2:D:746:GLU:OE2	2:D:746:GLU:N	2.38	0.45
1:G:500:ARG:O	1:G:501:SER:C	2.55	0.45
1:A:495:MET:HE2	1:A:512:LEU:CB	2.46	0.45
1:E:511:ASP:C	1:E:511:ASP:OD1	2.55	0.45
1:C:472:ASN:ND2	1:C:474:SER:H	2.15	0.45
2:D:656:ARG:HG3	2:D:785:ILE:HD11	1.98	0.45
1:A:413:GLU:HB3	4:A:2007:HOH:O	2.16	0.45
2:B:746:GLU:HG2	2:B:747:GLU:H	1.82	0.45
2:F:682:THR:HG23	2:F:780:SER:OG	2.17	0.45
2:B:719:LEU:HG	2:B:724:ILE:HD11	1.99	0.45
1:G:554:GLU:O	1:G:558:MET:HE2	2.17	0.45
1:C:523:LEU:HD23	4:C:2035:HOH:O	2.17	0.45
1:G:417:LYS:HB3	1:G:417:LYS:NZ	2.32	0.45
1:G:405:ASN:HD22	1:G:410:ASN:HD21	1.63	0.45
1:C:576:SER:O	1:C:578:ASP:N	2.49	0.45
2:F:785:ILE:O	2:F:786:PRO:C	2.55	0.45
1:C:435:GLY:H	1:C:508:SER:CA	2.26	0.45
1:G:480:ASN:HD21	1:G:484:MET:HE1	1.82	0.45
1:A:480:ASN:HD21	1:A:484:MET:HE1	1.82	0.45
1:E:420:LYS:O	1:E:420:LYS:HD3	2.16	0.45
1:G:512:LEU:CD2	1:G:517:ILE:H	2.30	0.44
1:E:472:ASN:HD22	1:E:474:SER:H	1.65	0.44
2:H:745:LYS:CB	2:H:745:LYS:NZ	2.79	0.44
2:H:678:HIS:CE1	2:H:779:LEU:HB3	2.52	0.44
2:F:681:TRP:O	2:F:685:GLN:HB2	2.17	0.44
1:C:512:LEU:HA	1:C:516:TRP:CB	2.44	0.44
1:G:389:LEU:HD12	1:G:389:LEU:HA	1.88	0.44
3:R:410:ASP:C	3:R:410:ASP:OD2	2.56	0.44
1:E:475:LYS:HZ2	3:R:426:ASP:HA	1.81	0.44
2:D:719:LEU:HD23	2:D:724:ILE:HD11	1.99	0.44
1:E:492:GLU:CD	1:E:512:LEU:HD11	2.37	0.44
1:G:574:LYS:HB3	1:G:574:LYS:NZ	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:SER:C	1:C:515:PRO:HD2	2.25	0.44
1:A:554:GLU:HG2	1:A:558:MET:CE	2.44	0.44
2:F:783:PRO:O	2:F:785:ILE:HD12	2.17	0.44
1:C:420:LYS:O	1:C:420:LYS:HE2	2.18	0.44
1:A:545:GLU:H	1:A:545:GLU:CD	2.20	0.44
2:F:775:ARG:N	2:F:776:PRO:HD3	2.33	0.44
2:B:683:LEU:HD12	2:B:711:ILE:HD13	1.98	0.44
1:C:576:SER:C	1:C:578:ASP:N	2.71	0.44
2:H:773:SER:C	2:H:775:ARG:H	2.21	0.44
2:F:761:MET:O	2:F:765:LYS:HB2	2.17	0.44
2:D:662:LEU:CD2	2:D:666:CYS:SG	3.06	0.44
2:B:694:LEU:HD12	2:B:694:LEU:HA	1.81	0.44
1:C:396:PRO:HG3	1:C:454:TYR:CE1	2.52	0.44
2:D:681:TRP:CD1	2:D:782:ILE:HD13	2.53	0.44
1:C:492:GLU:OE1	1:C:512:LEU:HD21	2.18	0.44
1:C:514:PHE:O	1:C:517:ILE:HG22	2.18	0.44
2:D:746:GLU:O	2:D:747:GLU:HG2	2.17	0.44
1:E:428:GLU:HB3	1:E:432:LYS:HZ3	1.79	0.43
1:A:430:PHE:HE2	1:A:495:MET:HE3	1.84	0.43
1:G:513:SER:HB3	1:G:515:PRO:HD2	1.99	0.43
1:G:387:MET:O	1:G:390:ASN:ND2	2.51	0.43
2:F:785:ILE:N	2:F:785:ILE:HD12	2.34	0.43
1:C:499:SER:O	1:C:501:SER:N	2.51	0.43
2:D:698:ARG:NH1	2:D:743:LEU:O	2.52	0.43
1:C:417:LYS:HE2	4:C:2010:HOH:O	2.18	0.43
1:G:432:LYS:HG3	4:G:2015:HOH:O	2.15	0.43
1:E:512:LEU:CD2	1:E:513:SER:O	2.66	0.43
1:E:434:VAL:HG12	1:E:434:VAL:O	2.18	0.43
2:B:660:LEU:HD21	2:B:785:ILE:CD1	2.49	0.43
2:F:665:LEU:HD12	2:F:665:LEU:HA	1.84	0.43
1:A:569:LEU:O	1:A:569:LEU:HD22	2.19	0.43
1:E:428:GLU:CB	1:E:432:LYS:HZ2	2.32	0.43
2:F:787:ARG:CD	2:F:787:ARG:N	2.81	0.43
2:D:711:ILE:HA	2:D:711:ILE:HD13	1.85	0.43
1:E:422:ILE:HD11	1:E:484:MET:CE	2.48	0.43
1:E:512:LEU:HD13	1:E:513:SER:C	2.39	0.42
1:E:436:GLN:C	1:E:438:CYS:H	2.21	0.42
1:A:512:LEU:HA	1:A:516:TRP:HB3	2.01	0.42
1:E:413:GLU:HG3	4:E:2010:HOH:O	2.16	0.42
1:A:440:GLU:HB3	1:G:511:ASP:OD2	2.20	0.42
1:G:434:VAL:HG21	1:G:511:ASP:OD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:691:GLU:CB	2:H:694:LEU:HD23	2.36	0.42
2:D:761:MET:O	2:D:765:LYS:N	2.49	0.42
1:E:422:ILE:HD11	1:E:484:MET:HE3	2.02	0.42
2:H:782:ILE:HD13	2:H:782:ILE:HA	1.92	0.42
2:F:683:LEU:HB2	2:F:711:ILE:HD11	2.01	0.42
1:C:434:VAL:O	1:C:435:GLY:C	2.57	0.42
1:G:486:LEU:HD23	1:G:531:VAL:HG21	2.01	0.42
1:C:554:GLU:HG2	1:C:558:MET:HE2	2.02	0.42
1:A:421:ASP:HB3	1:E:425:ILE:HD11	2.01	0.42
1:A:395:GLN:HE21	1:A:396:PRO:HD2	1.84	0.42
1:E:428:GLU:HB3	1:E:432:LYS:HZ2	1.83	0.42
2:F:757:ASN:HA	2:F:761:MET:HE3	2.02	0.42
3:R:409:LEU:HD12	3:R:410:ASP:HB3	2.01	0.42
1:G:475:LYS:CE	4:S:2005:HOH:O	2.67	0.42
3:S:417:GLU:CD	3:S:417:GLU:C	2.79	0.42
1:A:435:GLY:CA	1:A:508:SER:N	2.82	0.42
2:F:787:ARG:HD3	2:F:787:ARG:N	2.34	0.42
2:H:678:HIS:CD2	2:H:779:LEU:HD13	2.55	0.42
2:H:713:LYS:HA	4:H:2006:HOH:O	2.20	0.42
1:G:496:ALA:O	1:G:500:ARG:NH2	2.53	0.42
1:E:495:MET:CB	1:E:512:LEU:CB	2.98	0.42
3:R:416:GLU:HB2	3:R:419:GLU:HG3	2.01	0.42
2:H:721:PHE:CB	2:H:753:ILE:HD11	2.50	0.42
1:G:382:ILE:HD12	1:G:498:TYR:CE1	2.55	0.42
1:G:529:TYR:OH	2:H:649:LEU:HD12	2.20	0.42
1:C:514:PHE:CB	1:C:515:PRO:CD	2.98	0.42
1:G:434:VAL:O	1:G:434:VAL:CG1	2.68	0.42
1:E:499:SER:O	1:E:500:ARG:HB2	2.20	0.42
3:P:409:LEU:HD23	3:P:409:LEU:N	2.35	0.42
2:B:659:TYR:CE1	2:B:782:ILE:HD12	2.54	0.42
1:E:548:LYS:HE2	3:R:409:LEU:N	2.35	0.41
1:C:572:LEU:HA	1:C:572:LEU:HD12	1.86	0.41
1:G:428:GLU:HA	1:G:428:GLU:OE2	2.20	0.41
1:E:470:ILE:HD13	4:R:2003:HOH:O	2.21	0.41
1:A:380:ASN:OD1	1:A:384:GLN:NE2	2.53	0.41
1:C:567:SER:HA	1:C:568:PRO:HD3	1.92	0.41
1:G:441:ILE:O	1:G:445:ARG:HG3	2.19	0.41
2:F:743:LEU:HD23	2:F:749:TYR:CE1	2.55	0.41
2:D:787:ARG:NH1	2:D:787:ARG:HB3	2.35	0.41
1:G:575:GLN:OE1	1:G:575:GLN:HA	2.20	0.41
2:H:714:VAL:CG1	4:H:2005:HOH:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:GLY:N	1:C:508:SER:HA	2.31	0.41
1:C:496:ALA:HA	1:C:499:SER:HB2	2.03	0.41
1:G:472:ASN:ND2	1:G:472:ASN:C	2.73	0.41
2:F:678:HIS:CG	2:F:779:LEU:HD13	2.55	0.41
3:R:410:ASP:O	3:R:410:ASP:OD2	2.39	0.41
1:C:512:LEU:HD13	1:C:514:PHE:H	1.86	0.41
2:B:765:LYS:HB2	2:B:765:LYS:HZ2	1.86	0.41
1:G:492:GLU:OE2	1:G:512:LEU:HD11	2.21	0.41
1:A:470:ILE:HG23	1:A:472:ASN:H	1.85	0.41
2:F:645:THR:HG23	3:R:419:GLU:OE1	2.21	0.41
2:H:672:GLU:C	2:H:674:PRO:HD3	2.41	0.41
2:H:659:TYR:CE1	2:H:782:ILE:HD12	2.56	0.41
2:D:786:PRO:HB2	2:D:787:ARG:H	1.62	0.41
1:A:526:PHE:O	1:A:529:TYR:HD2	2.03	0.41
2:D:673:HIS:N	2:D:674:PRO:CD	2.83	0.41
1:E:557:ILE:CG2	1:E:562:ALA:HB2	2.51	0.41
1:A:420:LYS:C	1:A:420:LYS:HE2	2.41	0.41
1:E:437:GLY:HA2	4:E:2017:HOH:O	2.20	0.41
2:H:741:ARG:HG2	2:H:749:TYR:CD2	2.55	0.41
1:C:486:LEU:HA	1:C:486:LEU:HD23	1.87	0.41
2:F:736:GLN:HA	2:F:739:PHE:CE2	2.55	0.41
1:C:420:LYS:CE	4:C:2015:HOH:O	2.66	0.40
1:A:537:LYS:HE2	3:P:413:PHE:CD2	2.57	0.40
1:E:517:ILE:HG13	1:E:517:ILE:O	2.19	0.40
1:E:428:GLU:CG	1:E:432:LYS:HZ2	2.34	0.40
2:H:769:LEU:CD2	2:H:769:LEU:N	2.84	0.40
2:B:746:GLU:HG2	2:B:747:GLU:N	2.37	0.40
1:E:575:GLN:O	1:E:576:SER:C	2.60	0.40
2:F:784:HIS:C	2:F:786:PRO:HD2	2.42	0.40
2:H:728:TYR:C	2:H:730:ASP:H	2.23	0.40
2:F:727:ALA:O	2:F:730:ASP:HB2	2.21	0.40
1:E:526:PHE:O	1:E:529:TYR:HD2	2.05	0.40
3:S:421:ILE:CD1	3:S:425:PHE:HE1	2.35	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	190/218 (87%)	178 (94%)	6 (3%)	6 (3%)	5	8
1	C	190/218 (87%)	170 (90%)	14 (7%)	6 (3%)	5	8
1	E	190/218 (87%)	178 (94%)	10 (5%)	2 (1%)	17	36
1	G	190/218 (87%)	174 (92%)	10 (5%)	6 (3%)	5	8
2	B	142/152 (93%)	129 (91%)	11 (8%)	2 (1%)	14	28
2	D	142/152 (93%)	127 (89%)	13 (9%)	2 (1%)	14	28
2	F	142/152 (93%)	127 (89%)	11 (8%)	4 (3%)	6	10
2	H	142/152 (93%)	124 (87%)	15 (11%)	3 (2%)	9	16
3	P	16/18 (89%)	14 (88%)	2 (12%)	0	100	100
3	Q	16/18 (89%)	14 (88%)	1 (6%)	1 (6%)	2	2
3	R	16/18 (89%)	13 (81%)	1 (6%)	2 (12%)	0	0
3	S	16/18 (89%)	13 (81%)	2 (12%)	1 (6%)	2	2
All	All	1392/1552 (90%)	1261 (91%)	96 (7%)	35 (2%)	7	12

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	PHE
1	C	514	PHE
2	D	784	HIS
2	D	786	PRO
2	F	779	LEU
1	G	389	LEU
1	G	512	LEU
2	H	746	GLU
3	Q	410	ASP
3	R	416	GLU
1	A	440	GLU
1	A	512	LEU

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Mol	Chain	Res	Type
2	B	774	THR
2	B	786	PRO
1	C	499	SER
1	C	500	ARG
1	E	511	ASP
2	F	776	PRO
1	G	387	MET
1	G	511	ASP
2	H	784	HIS
3	R	417	GLU
1	A	472	ASN
1	A	473	PHE
1	C	510	THR
1	C	512	LEU
1	C	577	LYS
1	E	560	SER
2	F	786	PRO
1	G	388	ILE
1	A	513	SER
2	F	773	SER
3	S	410	ASP
1	G	560	SER
2	H	729	LYS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/200 (89%)	162 (91%)	16 (9%)	12	23
1	C	178/200 (89%)	163 (92%)	15 (8%)	14	26
1	E	178/200 (89%)	160 (90%)	18 (10%)	9	17
1	G	178/200 (89%)	163 (92%)	15 (8%)	14	26
2	B	139/147 (95%)	123 (88%)	16 (12%)	7	12
2	D	139/147 (95%)	127 (91%)	12 (9%)	13	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	139/147 (95%)	126 (91%)	13 (9%)	11	20
2	H	139/147 (95%)	129 (93%)	10 (7%)	18	35
3	P	15/15 (100%)	13 (87%)	2 (13%)	5	8
3	Q	15/15 (100%)	13 (87%)	2 (13%)	5	8
3	R	15/15 (100%)	11 (73%)	4 (27%)	0	1
3	S	15/15 (100%)	14 (93%)	1 (7%)	20	40
All	All	1328/1448 (92%)	1204 (91%)	124 (9%)	11	21

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	400	LEU
1	A	420	LYS
1	A	436	GLN
1	A	438	CYS
1	A	444	GLN
1	A	452	LEU
1	A	470	ILE
1	A	472	ASN
1	A	486	LEU
1	A	487	LEU
1	A	510	THR
1	A	523	LEU
1	A	529	TYR
1	A	548	LYS
1	A	569	LEU
1	A	576	SER
2	B	649	LEU
2	B	656	ARG
2	B	657	LEU
2	B	662	LEU
2	B	683	LEU
2	B	684	PHE
2	B	694	LEU
2	B	700	LEU
2	B	711	ILE
2	B	721	PHE
2	B	743	LEU
2	B	746	GLU
2	B	750	ASP

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Mol	Chain	Res	Type
2	B	769	LEU
2	B	770	GLN
2	B	787	ARG
1	C	400	LEU
1	C	420	LYS
1	C	436	GLN
1	C	438	CYS
1	C	452	LEU
1	C	472	ASN
1	C	484	MET
1	C	486	LEU
1	C	487	LEU
1	C	510	THR
1	C	517	ILE
1	C	519	ASN
1	C	523	LEU
1	C	529	TYR
1	C	569	LEU
2	D	657	LEU
2	D	662	LEU
2	D	683	LEU
2	D	684	PHE
2	D	685	GLN
2	D	696	ARG
2	D	700	LEU
2	D	721	PHE
2	D	743	LEU
2	D	746	GLU
2	D	750	ASP
2	D	784	HIS
1	E	383	GLN
1	E	389	LEU
1	E	399	ASN
1	E	413	GLU
1	E	428	GLU
1	E	436	GLN
1	E	452	LEU
1	E	466	GLU
1	E	467	ARG
1	E	472	ASN
1	E	486	LEU
1	E	487	LEU

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Mol	Chain	Res	Type
1	E	510	THR
1	E	511	ASP
1	E	513	SER
1	E	514	PHE
1	E	529	TYR
1	E	569	LEU
2	F	657	LEU
2	F	662	LEU
2	F	683	LEU
2	F	684	PHE
2	F	685	GLN
2	F	700	LEU
2	F	721	PHE
2	F	743	LEU
2	F	746	GLU
2	F	773	SER
2	F	775	ARG
2	F	786	PRO
2	F	787	ARG
1	G	399	ASN
1	G	413	GLU
1	G	424	TYR
1	G	428	GLU
1	G	429	LYS
1	G	436	GLN
1	G	452	LEU
1	G	466	GLU
1	G	472	ASN
1	G	484	MET
1	G	486	LEU
1	G	487	LEU
1	G	514	PHE
1	G	529	TYR
1	G	569	LEU
2	H	657	LEU
2	H	662	LEU
2	H	663	ASN
2	H	683	LEU
2	H	685	GLN
2	H	700	LEU
2	H	721	PHE
2	H	743	LEU

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Mol	Chain	Res	Type
2	H	745	LYS
2	H	787	ARG
3	P	409	LEU
3	P	422	ARG
3	Q	409	LEU
3	Q	422	ARG
3	R	409	LEU
3	R	416	GLU
3	R	417	GLU
3	R	422	ARG
3	S	417	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	383	GLN
1	A	384	GLN
1	A	395	GLN
1	A	405	ASN
1	A	436	GLN
1	A	472	ASN
1	A	478	ASN
1	A	480	ASN
1	A	541	ASN
1	A	555	HIS
2	B	678	HIS
2	B	685	GLN
2	B	689	GLN
2	B	733	HIS
2	B	762	GLN
2	B	770	GLN
1	C	383	GLN
1	C	384	GLN
1	C	395	GLN
1	C	405	ASN
1	C	436	GLN
1	C	472	ASN
1	C	480	ASN
1	C	541	ASN
1	C	555	HIS
2	D	689	GLN
2	D	733	HIS

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Mol	Chain	Res	Type
1	E	383	GLN
1	E	395	GLN
1	E	405	ASN
1	E	436	GLN
1	E	472	ASN
1	E	480	ASN
1	E	541	ASN
1	E	555	HIS
2	F	678	HIS
2	F	689	GLN
2	F	767	ASN
2	F	770	GLN
1	G	390	ASN
1	G	395	GLN
1	G	405	ASN
1	G	436	GLN
1	G	472	ASN
1	G	480	ASN
1	G	541	ASN
1	G	555	HIS
2	H	663	ASN
2	H	678	HIS
2	H	685	GLN
2	H	689	GLN
2	H	733	HIS
2	H	767	ASN
3	R	412	HIS
3	S	412	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	194/218 (88%)	0.04	7 (3%) 46 38	20, 29, 56, 74	0
1	C	194/218 (88%)	0.01	9 (4%) 36 29	20, 29, 55, 69	0
1	E	194/218 (88%)	0.19	11 (5%) 27 20	21, 30, 57, 77	0
1	G	194/218 (88%)	0.11	12 (6%) 24 18	21, 29, 58, 75	0
2	B	144/152 (94%)	0.40	15 (10%) 8 5	21, 38, 71, 79	0
2	D	144/152 (94%)	0.46	13 (9%) 12 8	24, 39, 72, 80	0
2	F	144/152 (94%)	0.59	17 (11%) 6 4	27, 43, 73, 80	0
2	H	144/152 (94%)	0.55	14 (9%) 10 6	27, 40, 72, 83	0
3	P	18/18 (100%)	0.88	4 (22%) 1 0	41, 48, 61, 64	0
3	Q	18/18 (100%)	0.85	4 (22%) 1 0	40, 49, 58, 61	0
3	R	18/18 (100%)	1.13	6 (33%) 0 0	39, 52, 65, 68	0
3	S	18/18 (100%)	1.22	5 (27%) 1 0	41, 51, 62, 64	0
All	All	1424/1552 (91%)	0.30	117 (8%) 14 10	20, 36, 65, 83	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	774	THR	9.2
2	D	774	THR	8.9
1	E	379	MET	7.9
2	B	776	PRO	7.3
2	H	787	ARG	7.3
2	B	774	THR	7.1
2	D	776	PRO	7.1
1	A	508	SER	6.4
3	S	409	LEU	6.2
2	F	776	PRO	6.1
2	H	786	PRO	6.0

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Mol	Chain	Res	Type	RSRZ
3	R	409	LEU	5.9
2	F	774	THR	5.7
2	B	786	PRO	5.6
1	G	379	MET	5.3
2	F	785	ILE	5.3
2	F	777	PRO	5.0
2	F	784	HIS	4.8
2	D	777	PRO	4.7
1	E	500	ARG	4.7
2	D	786	PRO	4.6
1	G	501	SER	4.6
2	D	775	ARG	4.6
1	C	510	THR	4.5
3	S	417	GLU	4.5
2	D	787	ARG	4.5
3	P	409	LEU	4.5
3	P	426	ASP	4.4
1	E	501	SER	4.4
2	H	785	ILE	4.3
2	H	773	SER	4.3
2	F	775	ARG	4.2
1	G	380	ASN	4.1
1	C	501	SER	4.1
2	B	787	ARG	4.0
1	A	501	SER	3.8
2	H	772	ALA	3.7
3	R	426	ASP	3.7
1	E	380	ASN	3.6
1	A	379	MET	3.6
2	F	787	ARG	3.6
2	F	773	SER	3.5
2	H	784	HIS	3.5
2	H	776	PRO	3.4
2	B	746	GLU	3.4
2	F	786	PRO	3.3
2	H	775	ARG	3.3
3	S	416	GLU	3.2
2	B	775	ARG	3.2
1	G	575	GLN	3.2
2	F	747	GLU	3.2
2	H	778	THR	3.2
3	R	417	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	773	SER	3.1
3	R	416	GLU	3.1
1	C	509	GLY	3.1
1	E	381	THR	3.1
3	Q	426	ASP	3.0
2	F	716	ASN	3.0
1	G	383	GLN	3.0
1	G	511	ASP	2.9
2	F	736	GLN	2.9
3	R	418	GLY	2.9
1	C	508	SER	2.8
2	D	746	GLU	2.8
2	F	730	ASP	2.7
1	E	390	ASN	2.7
1	E	578	ASP	2.7
1	C	512	LEU	2.7
3	Q	409	LEU	2.7
2	B	778	THR	2.6
2	D	784	HIS	2.6
3	Q	410	ASP	2.6
1	C	500	ARG	2.6
2	B	785	ILE	2.6
2	F	780	SER	2.6
1	E	575	GLN	2.6
2	F	668	ARG	2.5
2	H	716	ASN	2.5
3	R	410	ASP	2.5
2	B	718	ASP	2.5
2	B	777	PRO	2.5
3	P	410	ASP	2.4
1	C	436	GLN	2.4
1	A	509	GLY	2.4
1	G	388	ILE	2.4
2	D	778	THR	2.4
1	A	510	THR	2.4
2	B	736	GLN	2.4
2	D	773	SER	2.3
1	E	387	MET	2.3
3	P	418	GLY	2.3
3	S	410	ASP	2.3
2	B	784	HIS	2.3
2	F	745	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	576	SER	2.3
2	F	714	VAL	2.3
2	H	747	GLU	2.3
1	A	500	ARG	2.3
1	E	544	ARG	2.3
2	D	745	LYS	2.2
1	C	511	ASP	2.2
2	B	781	PRO	2.2
3	Q	418	GLY	2.2
2	D	779	LEU	2.2
1	G	381	THR	2.2
1	E	513	SER	2.2
2	H	781	PRO	2.1
1	C	513	SER	2.1
1	G	513	SER	2.1
3	S	418	GLY	2.1
2	D	785	ILE	2.1
1	G	391	SER	2.1
2	H	777	PRO	2.0
1	A	578	ASP	2.0
1	G	390	ASN	2.0
2	B	779	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.